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Contents

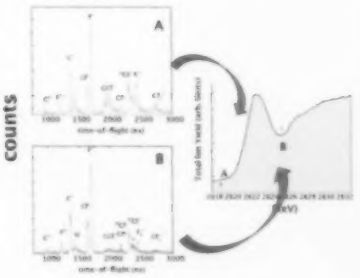
Articles

1–8

Deep core ionic photofragmentation of the CF_2Cl_2 molecule

A.H.A. Gomes, W. Wolff, N. Ferreira, K.F. Alcantara, H. Luna, G.M. Sigaud, A.C.F. Santos

► The photoionization of the CF_2Cl_2 molecule has been studied around the Cl K edge. ► Photoion yields for the fragmentation products have been recorded. ► The CF_2Cl_2 undergoes a full break up with the formation of doubly charged fragments. ► A relative site-selective fragmentation can be observed.

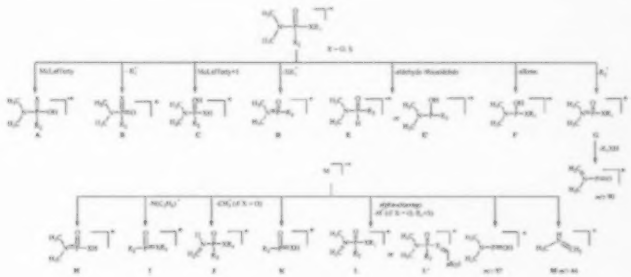


9–16

Mass spectrometric study on *o*(*s*)-alkyl *N*,*N*-dimethylamino alkylphosphonates (alkylphosphonothiolates) for Chemical Weapons Convention verification purposes

Hamdollah Saeidian, Davood Ashrafi, Mansour Sarabadani, Mohammad Taghi Naseri, Mehran Babri

► Modified microsynthesis of *O*(*S*)-alkyl *N*,*N*-dimethylamino alkylphosphonates (alkylphosphonothiolates) which are included in schedule 2 of Chemical Weapons Convention (CWC) annex of chemicals, is reported. ► Their electron impact mass spectra with possible fragmentation routes are also investigated by MS/MS experiments, fragment ions of deuterated analogs and energy calculations. ► These data could be useful for successful detection and identification the CWC-related chemicals in real sample or during OPCW proficiency tests.

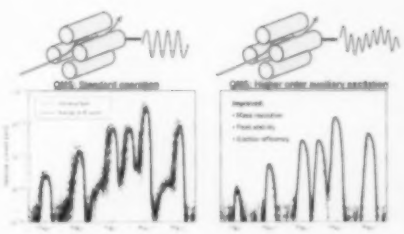


17–24

Comparing the performance of hyperbolic and circular rod quadrupole mass spectrometers with applied higher order auxiliary excitation

D.J. Gershman, B.P. Block, M. Rubin, M. Benna, P.R. Mahaffy, T.H. Zurbuchen

► We apply higher order auxiliary excitation to quadrupole mass spectrometers. ► Mass resolution, stability, and peak shape improve for circular rod sensors. ► Stability and ion peak shape improve for hyperbolic rod sensors.



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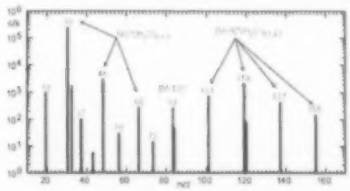
http://dx.doi.org/10.1016/S1387-3806(12)00215-1

25–30

A selected ion flow tube study of the reactions of H_3O^+, NO^+ and $O_2^{+\bullet}$ with seven isomers of hexanol in support of SIFT-MS

David Smith, Kristýna Sovová, Patrik Španěl

▶ Dissociative proton transfer from H_3O^+ produces $C_6H_{13}^+$ ions only. ▶ Hydride ion transfer to NO^+ produces mostly $C_6H_{13}O^+$ ions that associate with H_2O with varied rates. ▶ $O_2^{+\bullet}$ reacts by dissociative charge transfer analogous to electron ionization. ▶ Rate constants useful for absolute quantification of the total concentration of all hexanol are similar for different isomers. ▶ Quantification of various isomers of hexanol in the vapours emitted from foods and other products is therefore possible by SIFT-MS.

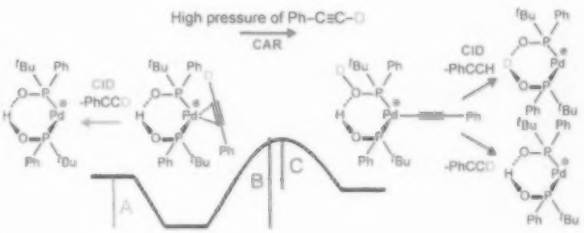


31–39

RRKM modeling of collision activated reaction/collision induced dissociation experiments: Energy profile determination for phenylethyne incorporation on palladium (II)–phosphinous acid complex

Denis Lesage, Antony Memboeuf, Yves Gimbert, Jean-Claude Tabet

▶ We present a RRKM modeling of the coordination of phenylethyne on a Pd(II) phosphinous acid complex. ▶ Two structures are formed under high pressure collision activated reaction (CAR). ▶ Deuterated phenylethyne is used to differentiate these two structures. ▶ Energy profile for isomerization and decomposition processes is determined.

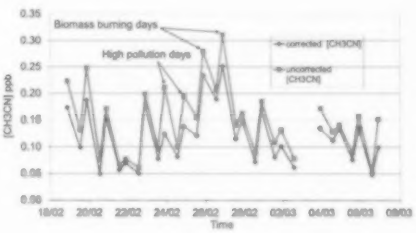


40–47

Interference in the PTR-MS measurement of acetonitrile at *m/z* 42 in polluted urban air—A study using switchable reagent ion PTR-MS

Erin Dunne, Ian E. Galbally, Sarah Lawson, Antonio Patti

▶ PTR-MS measurements of acetonitrile in urban air. ▶ SRI + PTR-MS used for discrimination of acetonitrile signal at *m/z* 42 from interfering ion signals $C_3H_6^+$ and $^{13}C^{12}C_2H_5^+$. ▶ Interference constituted 5–41% of *m/z* 42 ion signal observed in urban air. ▶ Corrected acetonitrile concentration a more sensitive tracer for biomass burning.

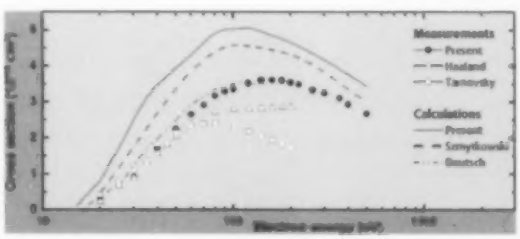


48–54

Electron ionization of NF_3

M.A. Rahman, Sumona Gangopadhyay, Chetan Limbachiya, K.N. Joshipura, E. Krishnakumar

▶ Partial and total electron impact ionization cross sections for NF_3 are measured. ▶ Total scattering and total ionization cross sections are also calculated. ▶ Measurements differ considerably from previous measurements and present calculations. ▶ The measured cross sections agree well with the "new" Deutsch–Mark additivity rule. ▶ The appearance potentials for various ions are measured, estimated and compared.

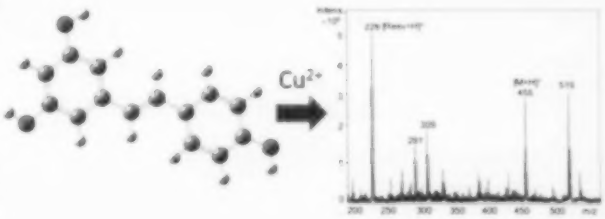


55–63

A joint experimental and theoretical investigation on the oxidative coupling of resveratrol induced by copper and iron ions

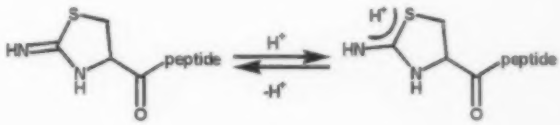
Vajir F. Tamboli, Nazzareno Re, Cecilia Coletti, Andrea Defant, Ines Mancini, Paolo Tosi

► The first ESI-MS study of the oxidative coupling of resveratrol induced by copper and iron ions. ► Copper ions induce the production of racemic δ-viniferin, iron ions give isomeric racemic ε-viniferin. ► Reaction mechanisms have been investigated by DFT calculations.



64–67

Method for enhancing peptide signal in time-of-flight secondary ion mass spectrometry

Junpei Naito, Shuya Satoh, Yoichi Otsuka, Hiroyuki Hashimoto

► We modified peptides containing only one cysteine at the N-terminus with NTCB. ► The modified peptide achieves high sensitivity for TOF-SIMS detection. ► It seems that it is due to the proton affinity of the modified N-terminus.